SUPPLEMENTARY FIGURES: Critical Assessment of Methods of Protein Structure Prediction (CASP) – Round XII
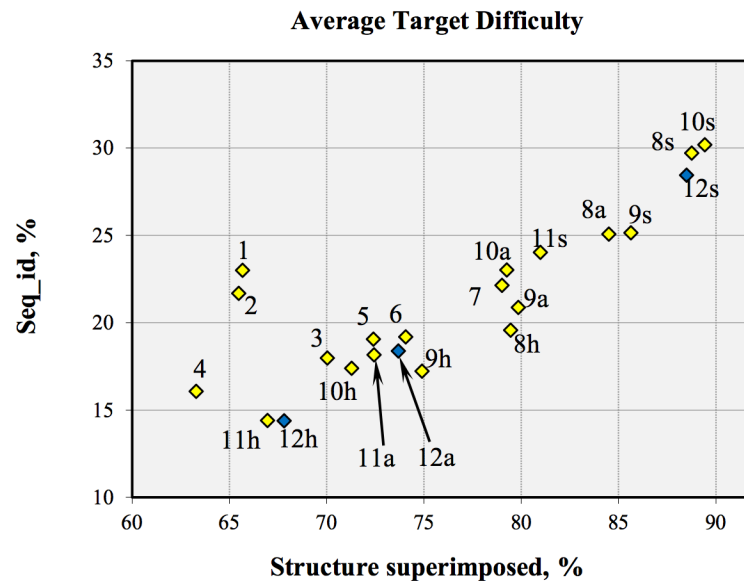

Figure S1. Average target difficulty in each CASP experiment, expressed as the average fraction of each target that superimposes on the closest structural template (X-axis) and the average sequence identity to that template (Y axis). The lower and further to the left a CASP point lies, the harder the target. For CASP12, the most recent experiment, the average for all targets ('12a') is very similar to that of CASP11. In recent CASPs, targets are divided into two subsets: targets which were only released for servers ('s'), and targets where all methods may be used ('h'). The Server set in CASP12 was relatively easy ('12s' near the top right) while the all methods set (12h) was one of the hardest in all CASPs, and similar to that of CASP11 (11h).
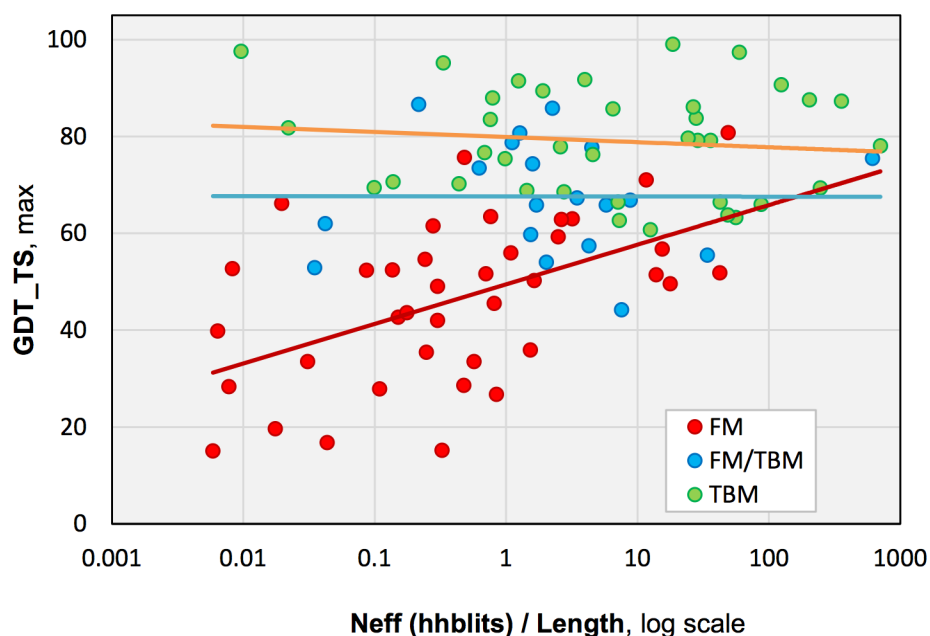
Figure S2: Backbone accuracy of the best model for each target as a function of the length-normalized alignment depth. Accuracy is strongly dependent on alignment depth for free modeling (FM) targets, indicating that predicted contacts make a major contribution. For targets where templates were used, this is not the case – there is no apparent improvement from incorporating predicted contact information. Neff is the number of diverse (less than 90% ID) homologous sequences covering at least 60% of the target with an E-score of 10^{-3} or better, retrieved by HHblits from the uniprot20 database.
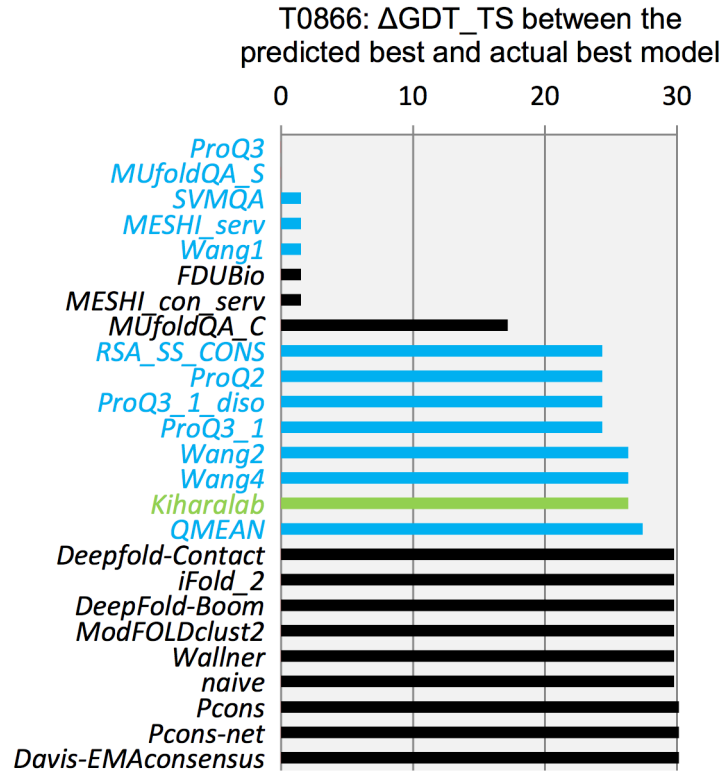
Figure S3: Performance of methods for estimating model accuracy (EMA) for target T0866: Difference in GDT_TS scores between the best predicted model and the model with the highest EMA score, for the 25 top ranking EMA methods. Single-model methods are blue, quasi-single green, and clustering methods black. Two single-model EMA methods correctly identified the most accurate model, while the next five suggested the second most accurate model as the best (difference in the GDT_TS scores of 1.5). For this target and overall, CASP12 single model methods were more accurate than clustering approaches.
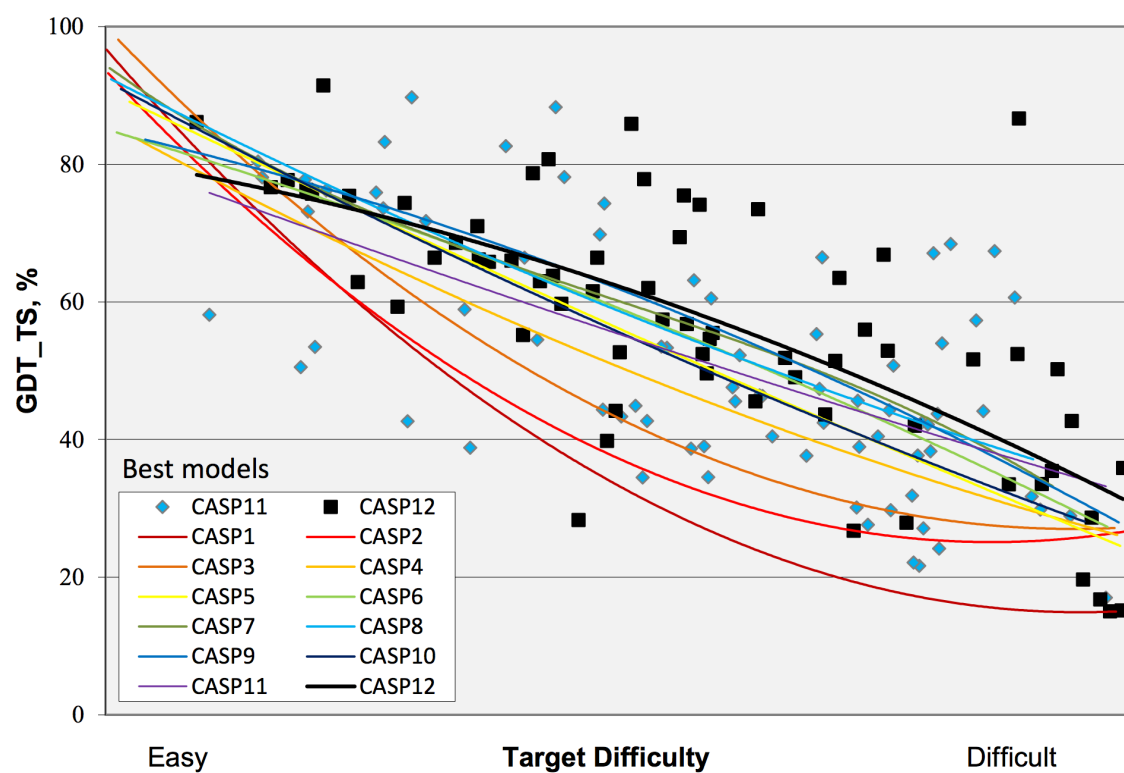
Figure S4: Best model backbone accuracy (GDT_TS) trend lines for each CASP. Over the course of the CASP experiments accuracy has increased dramatically. Individual target data points are shown for the two most recent CASPs.